UNIVERSITY OF WASHINGTON

Introduction to Boosted Trees

Tianqi Chen

Oct. 22 2014

Outline

- **Review of key concepts of supervised learning**
- Regression Tree and Ensemble (What are we Learning)
- Gradient Boosting (How do we Learn)
- Summary

Elements in Supervised Learning

- Notations: $x_i \in \mathbf{R}^d$ i-th training example
- **Model**: how to make prediction $\hat{y}_i$ given x_i
  - Linear model: $\hat{y}_i = \sum_j w_j x_{ij}$ (include linear/logistic regression)
  - The prediction score $\hat{y}_i$ can have different interpretations depending on the task
    - Linear regression: $\hat{y}_i$ is the predicted score
    - Logistic regression: $1/(1+exp(-\hat{y}_i))$ is predicted the probability of the instance being positive
    - Others… for example in ranking $\hat{y}_i$ can be the rank score
- **Parameters**: the things we need to learn from data
  - Linear model: $\Theta = \{w_j | j = 1, \cdots, d\}$

Elements continued: Objective Function

- Objective function that is everywhere

$$Obj(\Theta) = L(\Theta) + \Omega(\Theta)$$

Training Loss measures how well model fit on training data

Regularization, measures complexity of model

- Loss on training data: $L = \sum_{i=1}^{n} l(y_i, \hat{y}_i)$
  - Square loss: $l(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$
  - Logistic loss: $l(y_i, \hat{y}_i) = y_i \ln(1 + e^{-\hat{y}_i}) + (1 - y_i) \ln(1 + e^{\hat{y}_i})$
- Regularization: how complicated the model is?
  - L2 norm: $\Omega(w) = \lambda \|w\|^2$
  - L1 norm (lasso): $\Omega(w) = \lambda \|w\|_1$

Putting known knowledge into context

- Ridge regression: $\sum_{i=1}^{n}(y_i - w^T x_i)^2 + \lambda\|w\|^2$
  - Linear model, square loss, L2 regularization
- Lasso: $\sum_{i=1}^{n}(y_i - w^T x_i)^2 + \lambda\|w\|_1$
  - Linear model, square loss, L1 regularization
- Logistic regression:

$$\sum_{i=1}^{n}[y_i \ln(1 + e^{-w^T x_i}) + (1 - y_i)\ln(1 + e^{w^T x_i})] + \lambda\|w\|^2$$

  - Linear model, logistic loss, L2 regularization
- The conceptual separation between model, parameter, objective also gives you **engineering benefits**.
  - Think of how you can implement SGD for both ridge regression and logistic regression

Objective and Bias Variance Trade-off

$$Obj(\Theta) = L(\Theta) + \Omega(\Theta)$$

Training Loss measures how well model fit on training data

Regularization, measures complexity of model

- Why do we want to contain two component in the objective?
- Optimizing training loss encourages **predictive** models
  - Fitting well in training data at least get you close to training data which is hopefully close to the underlying distribution
- Optimizing regularization encourages **simple** models
  - Simpler models tends to have smaller variance in future predictions, making prediction **stable**

Outline

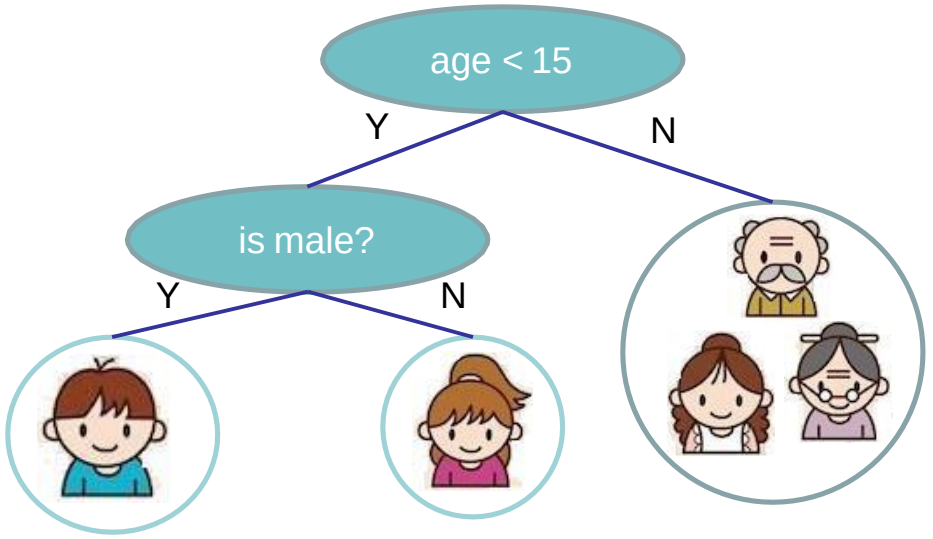
- Review of key concepts of supervised learning
- **Regression Tree and Ensemble (What are we Learning)**
- Gradient Boosting (How do we Learn)
- Summary

Regression Tree (CART)

- regression tree (also known as classification and regression tree):
  - Decision rules same as in decision tree
  - Contains one score in each leaf value

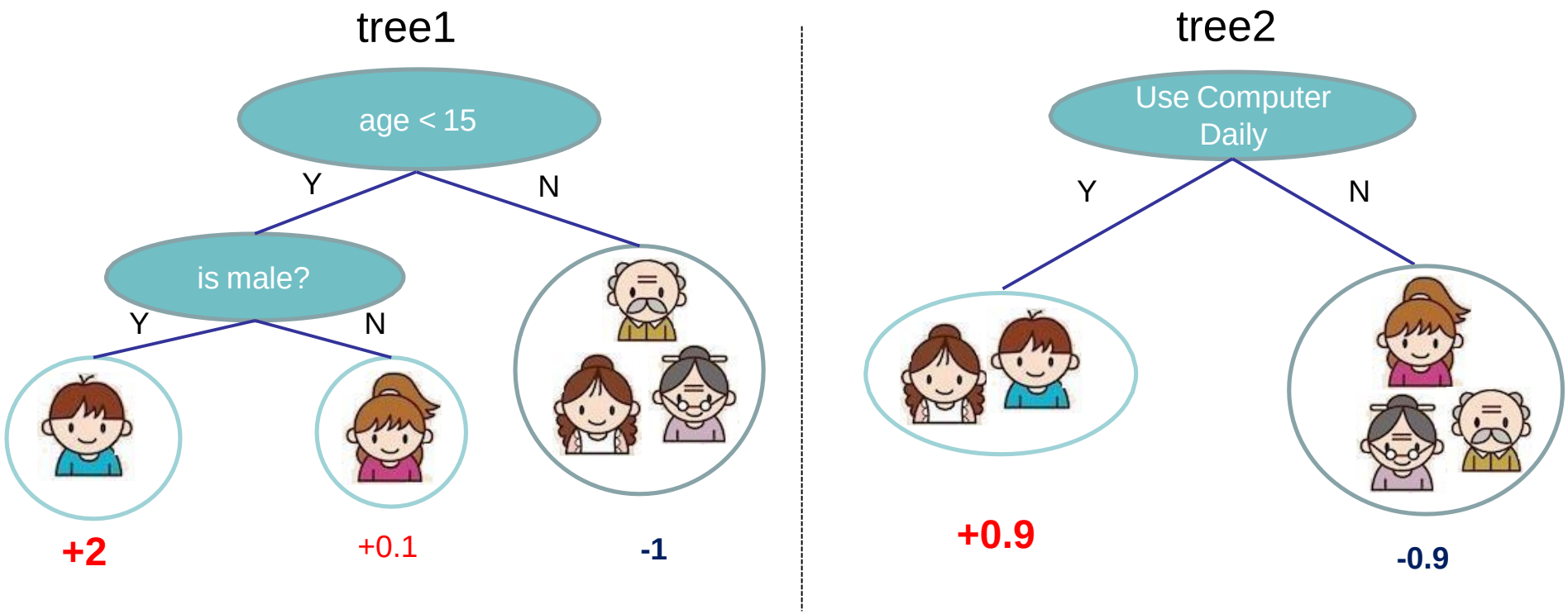
Input: age, gender, occupation, …

Does the person like computer games



prediction score in each leaf → **+2** +0.1 **-1**

Regression Tree Ensemble



f() = 2 + 0.9= 2.9

f()= -1 - 0.9= -1.9

Prediction of is sum of scores predicted by each of the tree

Tree Ensemble methods

- Very widely used, look for GBM, random forest…
  - Almost half of data mining competition are won by using some variants of tree ensemble methods
- Invariant to scaling of inputs, so you do not need to do careful features normalization.
- Learn higher order interaction between features.
- Can be scalable, and are used in Industry

Put into context: Model and Parameters

- Model: assuming we have K trees

$$\hat{y}_i = \sum_{k=1}^{K} f_k(x_i), \quad f_k \in \mathcal{F}$$

Space of functions containing all Regression trees

Think: regression tree is a function that maps the attributes to the score

- Parameters
  - Including structure of each tree, and the score in the leaf
  - Or simply use function as parameters

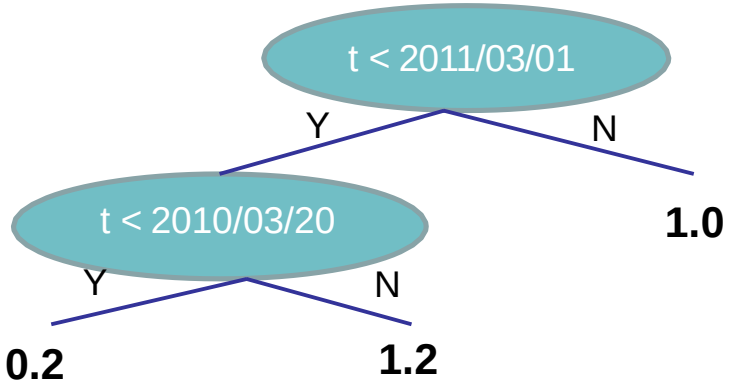
$$\Theta = \{f_1, f_2, \cdots, f_K\}$$

  - Instead learning weights in $\mathbf{R}^d$, we are learning functions(trees)

Learning a tree on single variable

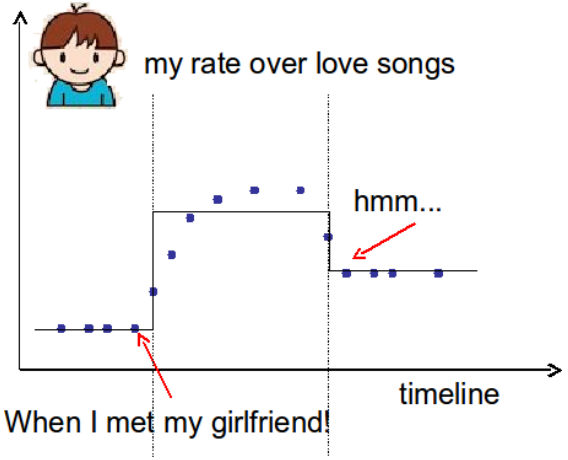
- How can we learn functions?
- Define objective (loss, regularization), and optimize it!!
- Example:
  - Consider regression tree on single input t (time)
  - I want to predict whether I like romantic music at time t

The model is regression tree that splits on time



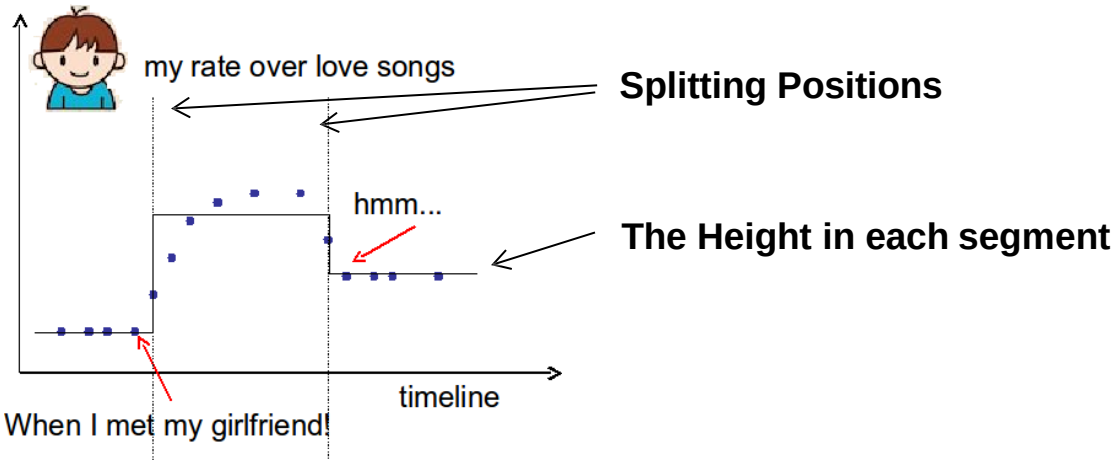
Equivalently

Piecewise step function over time



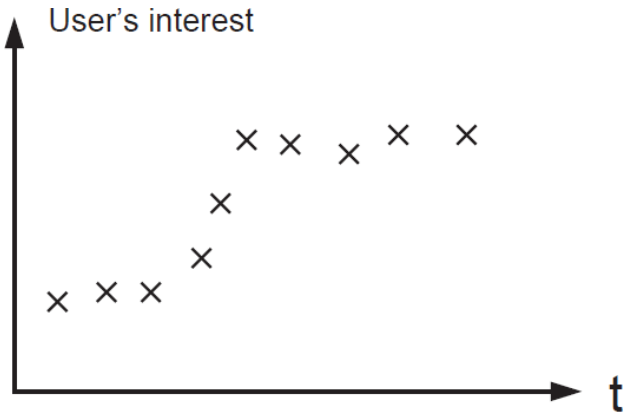
Learning a step function

- Things we need to learn

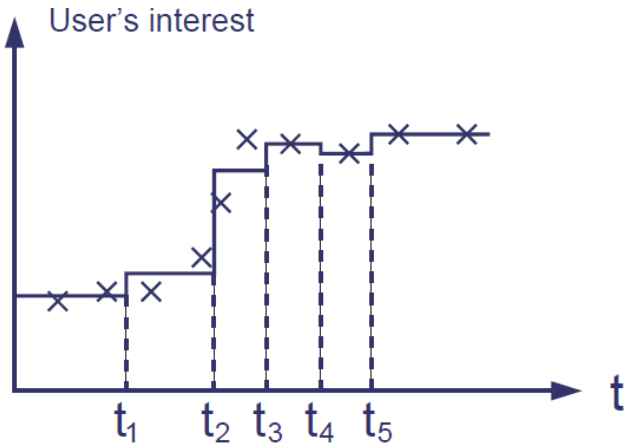


- Objective for single variable regression tree(step functions)
  - Training Loss: How will the function fit on the points?
  - Regularization: How do we define complexity of the function?
    - Number of splitting points, l2 norm of the height in each segment?

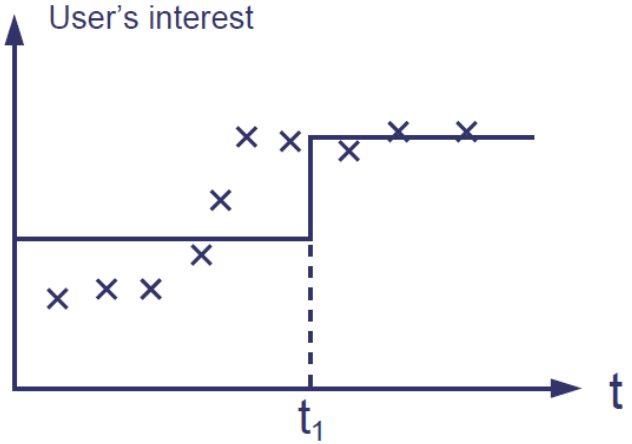
Learning step function (visually)



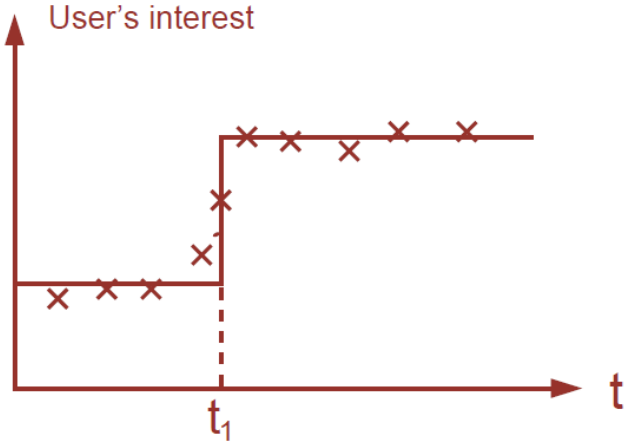
Observed user's interest on topic k against time t



☒ Too many splits, $\Omega(f)$ is high



☒ Wrong split point, $L(f)$ is high



☑ Good balance of $\Omega(f)$ and $L(f)$

Coming back: Objective for Tree Ensemble

- Model: assuming we have K trees

$$\hat{y}_i = \sum_{k=1}^{K} f_k(x_i), \quad f_k \in \mathcal{F}$$

- Objective

$$Obj = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k)$$

Training loss

Complexity of the Trees

- Possible ways to define Ω ?
  - Number of nodes in the tree, depth
  - L2 norm of the leaf weights
  - …detailed later

Objective vs Heuristic

- When you talk about (decision) trees, it is usually heuristics
  - Split by information gain
  - Prune the tree
  - Maximum depth
  - Smooth the leaf values
- Most heuristics maps well to objectives, taking the formal (objective) view let us know what we are learning
  - Information gain -> training loss
  - Pruning -> regularization defined by #nodes
  - Max depth -> constraint on the function space
  - Smoothing leaf values -> L2 regularization on leaf weights

Regression Tree is not just for regression!

- Regression tree ensemble defines how you make the prediction score, it can be used for
  - Classification, Regression, Ranking….
  - ….
- It all depends on how you define the objective function!
- So far we have learned:
  - Using Square loss $l(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$
    - Will results in common gradient boosted machine
  - Using Logistic loss $l(y_i, \hat{y}_i) = y_i \ln(1 + e^{-\hat{y}_i}) + (1 - y_i) \ln(1 + e^{\hat{y}_i})$
    - Will results in LogitBoost

Outline

- Review of key concepts of supervised learning
- Regression Tree and Ensemble (What are we Learning)
- **Gradient Boosting (How do we Learn)**
- Summary

Take Home Message for this section

- Bias-variance tradeoff is everywhere
- The loss + regularization objective pattern applies for regression tree learning (function learning)

- We want **predictive** and **simple** functions

- This defines what we want to learn (objective, model).
- But how do we learn it?
  - Next section

So How do we Learn?

- Objective: $\sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_k \Omega(f_k), f_k \in \mathcal{F}$
- We can not use methods such as SGD, to find f (since they are trees, instead of just numerical vectors)
- Solution: **Additive Training (Boosting)**
  - Start from constant prediction, add a new function each time

$$
\begin{aligned}
\hat{y}_i^{(0)} &= 0 \\
\hat{y}_i^{(1)} &= f_1(x_i) = \hat{y}_i^{(0)} + f_1(x_i) \\
\hat{y}_i^{(2)} &= f_1(x_i) + f_2(x_i) = \hat{y}_i^{(1)} + f_2(x_i) \\
&\cdots \\
\hat{y}_i^{(t)} &= \sum_{k=1}^{t} f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i)
\end{aligned}
$$

New function

Model at training round t

Keep functions added in previous round

Additive Training

- How do we decide which f to add?
  - Optimize the objective!!
- The prediction at round t is $\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + f_t(x_i)$

This is what we need to decide in round t

$$\begin{aligned} Obj^{(t)} &= \sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t)}) + \sum_{i=1}^{t} \Omega(f_i) \\ &= \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + constant \end{aligned}$$

Goal: find f_t to minimize this

- Consider square loss

$$\begin{aligned} Obj^{(t)} &= \sum_{i=1}^{n} \left(y_i - (\hat{y}_i^{(t-1)} + f_t(x_i))\right)^2 + \Omega(f_t) + const \\ &= \sum_{i=1}^{n} \left[2(\hat{y}_i^{(t-1)} - y_i) f_t(x_i) + f_t(x_i)^2\right] + \Omega(f_t) + const \end{aligned}$$

This is usually called residual from previous round

Taylor Expansion Approximation of Loss

- Goal $Obj^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + constant$
  - Seems still complicated except for the case of square loss
- Take Taylor expansion of the objective
  - Recall $f(x + \Delta x) \simeq f(x) + f'(x)\Delta x + \frac{1}{2} f''(x)\Delta x^2$
  - Define $g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial^2_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$

$$Obj^{(t)} \simeq \sum_{i=1}^{n} \left[l(y_i, \hat{y}_i^{(t-1)}) + g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t) + constant$$

- *If you are not comfortable with this, think of square loss*

$$g_i = \partial_{\hat{y}^{(t-1)}} (\hat{y}^{(t-1)} - y_i)^2 = 2(\hat{y}^{(t-1)} - y_i) \quad h_i = \partial^2_{\hat{y}^{(t-1)}} (y_i - \hat{y}^{(t-1)})^2 = 2$$

- Compare what we get to previous slide

Our New Goal

- Objective, with constants removed

$$\sum_{i=1}^{n} \left[g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t)$$

  - where $g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial^2_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$

- Why spending s much efforts to derive the objective, why not just grow trees …
  - Theoretical benefit: know what we are learning, convergence
  - **Engineering** benefit, recall the elements of supervised learning
    - g_i and h_i comes from definition of loss function
    - The learning of function only depend on the objective via g_i and h_i
    - Think of how you can separate modules of your code when you are asked to implement boosted tree for both square loss and logistic loss

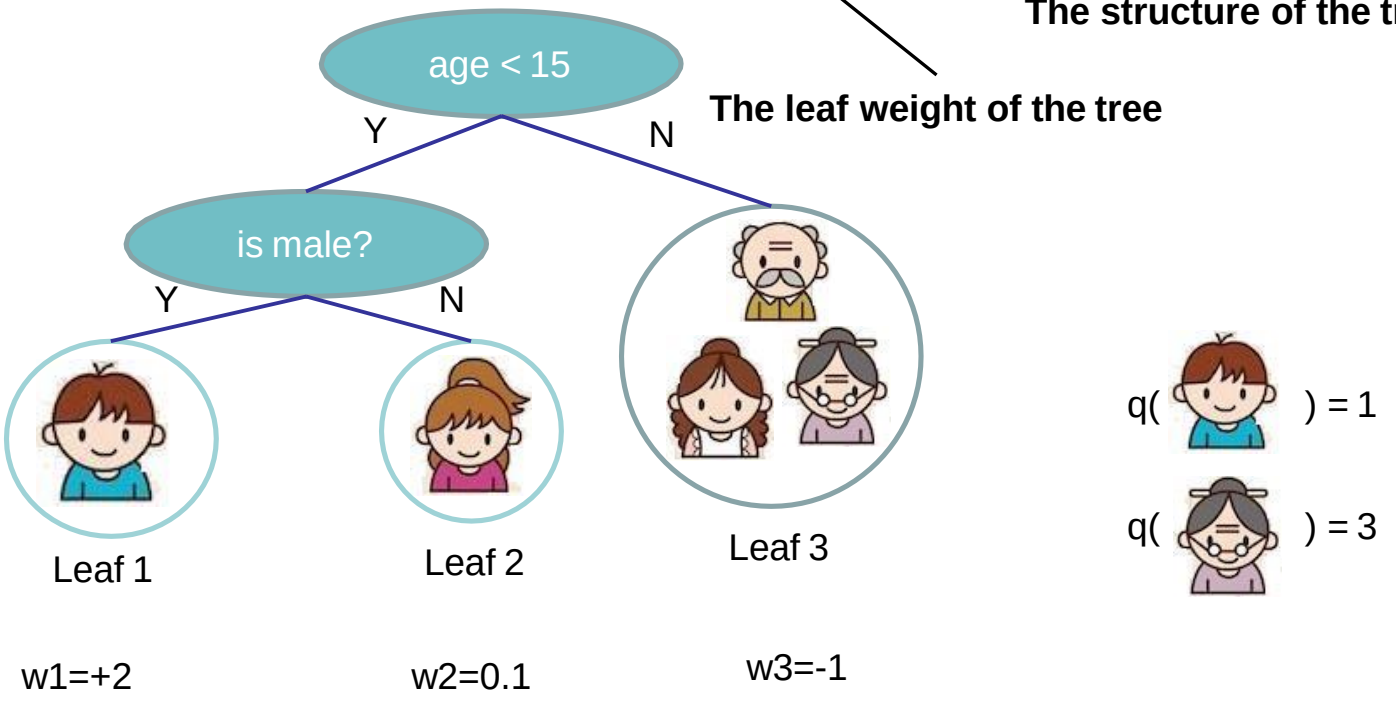
Refine the definition of tree

- We define tree by a vector of scores in leafs, and a leaf index mapping function that maps an instance to a leaf

$$f_t(x) = w_{q(x)}, \quad w \in \mathbf{R}^T, q : \mathbf{R}^d \rightarrow \{1, 2, \cdots, T\}$$

The structure of the tree

The leaf weight of the tree

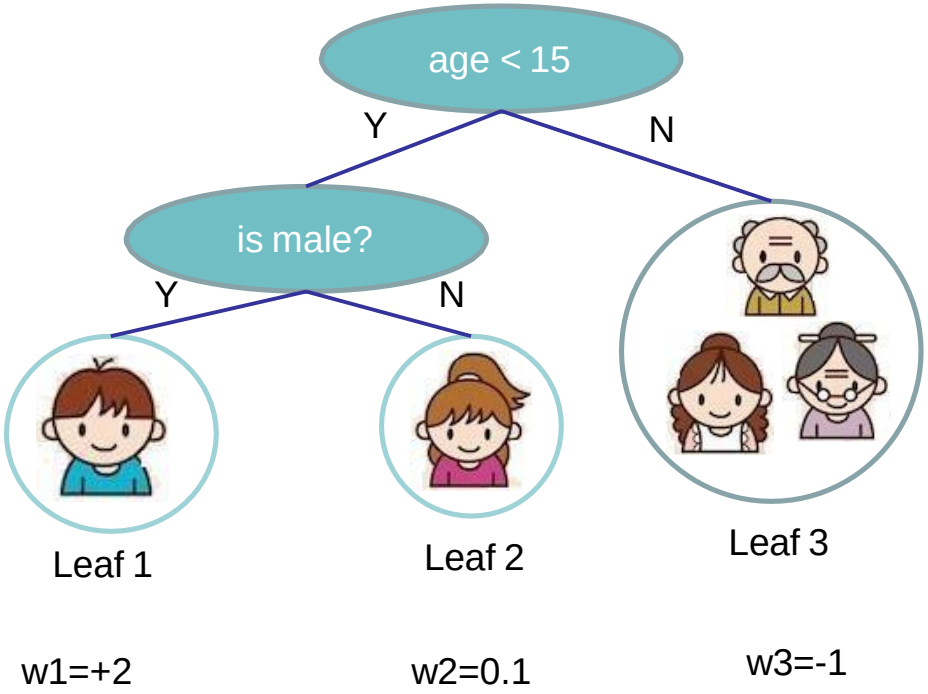


Define Complexity of a Tree (cont')

- Define complexity as (this is not the only possible definition)

$$\Omega(f_t) = \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} w_j^2$$

Number of leaves **L2 norm of leaf scores**



$$\Omega = \gamma 3 + \frac{1}{2}\lambda(4 + 0.01 + 1)$$

Revisit the Objectives

- Define the instance set in leaf j as $I_j = \{i|q(x_i) = j\}$
- Regroup the objective by each leaf

$$
\begin{aligned}
Obj^{(t)} &\simeq \sum_{i=1}^{n} \left[g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t) \\
&= \sum_{i=1}^{n} \left[g_i w_{q(x_i)} + \frac{1}{2} h_i w_{q(x_i)}^2 \right] + \gamma T + \lambda \frac{1}{2} \sum_{j=1}^{T} w_j^2 \\
&= \sum_{j=1}^{T} \left[(\sum_{i \in I_j} g_i) w_j + \frac{1}{2} (\sum_{i \in I_j} h_i + \lambda) w_j^2 \right] + \gamma T
\end{aligned}
$$

- This is sum of T independent quadratic functions

The Structure Score

- Two facts about single variable quadratic function

$$argmin_x \; Gx + \tfrac{1}{2}Hx^2 = -\tfrac{G}{H}, \; H > 0 \qquad \min_x \; Gx + \tfrac{1}{2}Hx^2 = -\tfrac{1}{2}\tfrac{G^2}{H}$$

- Let us define $G_j = \sum_{i \in I_j} g_i \quad H_j = \sum_{i \in I_j} h_i$

$$\begin{aligned} Obj^{(t)} &= \sum_{j=1}^{T} \left[(\sum_{i \in I_j} g_i) w_j + \tfrac{1}{2} (\sum_{i \in I_j} h_i + \lambda) w_j^2 \right] + \gamma T \\ &= \sum_{j=1}^{T} \left[G_j w_j + \tfrac{1}{2} (H_j + \lambda) w_j^2 \right] + \gamma T \end{aligned}$$

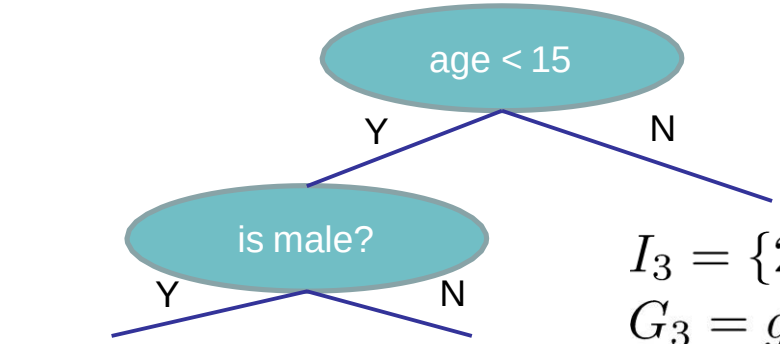
- Assume the structure of tree (q(x)) is fixed, the optimal weight in each leaf, and the resulting objective value are

$$w_j^* = -\frac{G_j}{H_j + \lambda} \qquad Obj = -\tfrac{1}{2} \sum_{j=1}^{T} \frac{G_j^2}{H_j + \lambda} + \gamma T$$

This measures how good a tree structure is!

The Structure Score Calculation

Instance index		gradient statistics
1		g1, h1
2		g2, h2
3		g3, h3
4		g4, h4
5		g5, h5



$$I_1 = \{1\} \quad G_1 = g_1 \quad H_1 = h_1$$

$$I_2 = \{4\} \quad G_2 = g_4 \quad H_4 = h_4$$

$$I_3 = \{2, 3, 5\} \quad G_3 = g_2 + g_3 + g_5 \quad H_3 = h_2 + h_3 + h_5$$

$$Obj = -\sum_j \frac{G_j^2}{H_j + \lambda} + 3\gamma$$

The smaller the score is, the better the structure is

Searching Algorithm for Single Tree

- Enumerate the possible tree structures q
- Calculate the structure score for the q, using the scoring eq.

$$Obj = -\frac{1}{2}\sum_{j=1}^{T}\frac{G_j^2}{H_j+\lambda} + \gamma T$$

- Find the best tree structure, and use the optimal leaf weight

$$w_j^* = -\frac{G_j}{H_j+\lambda}$$

- But…there can be infinite possible tree structures..

Greedy Learning of the Tree

- In practice, we grow the tree greedily
  - Start from tree with depth 0
  - For each leaf node of the tree, try to add a split. The change of objective after adding the split is

$$Gain = \frac{1}{2}\left[\frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{(G_L+G_R)^2}{H_L+H_R+\lambda}\right] - \gamma$$

The complexity cost by introducing additional leaf

the score of left child

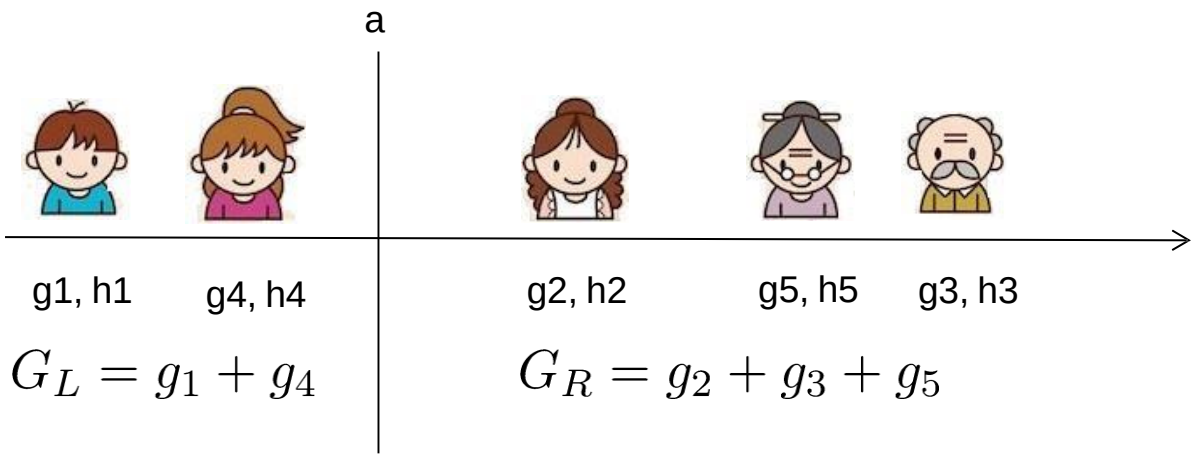
the score of right child

the score of if we do not split

  - Remaining question: how do we find the best split?

Efficient Finding of the Best Split

- What is the gain of a split rule $x_j < a$? Say x_j is age



- All we need is sum of g and h in each side, and calculate

$$Gain = \frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{(G_L+G_R)^2}{H_L+H_R+\lambda} - \gamma$$

- Left to right linear scan over sorted instance is enough to decide the best split along the feature

An Algorithm for Split Finding

- For each node, enumerate over all features
  - For each feature, sorted the instances by feature value
  - Use a linear scan to decide the best split along that feature
  - Take the best split solution along all the features

- Time Complexity growing a tree of depth K
  - It is O(n d K log n): or each level, need O(n log n) time to sort There are d features, and we need to do it for K level
  - This can be further optimized (e.g. use approximation or caching the sorted features)
  - Can scale to very large dataset

What about Categorical Variables?

- Some tree learning algorithm handles categorical variable and continuous variable separately
  - We can easily use the scoring formula we derived to score split based on categorical variables.
- Actually it is not necessary to handle categorical separately.
  - We can encode the categorical variables into numerical vector using one-hot encoding. Allocate a #categorical length vector

$$z_j = \begin{cases} 1 & \text{if } x \text{ is in category } j \\ 0 & otherwise \end{cases}$$

  - The vector will be sparse if there are lots of categories, the learning algorithm is preferred to handle sparse data

Pruning and Regularization

- Recall the gain of split, it can be negative!

$$Gain = \frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{(G_L+G_R)^2}{H_L+H_R+\lambda} - \gamma$$

  - When **the training loss reduction** is smaller than **regularization**
  - Trade-off between simplicity and predictivness
- Pre-stopping
  - Stop split if the best split have negative gain
  - But maybe a split can benefit future splits..
- Post-Prunning
  - Grow a tree to maximum depth, recursively prune all the leaf splits with negative gain

Recap: Boosted Tree Algorithm

- Add a new tree in each iteration
- Beginning of each iteration, calculate

$$g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial^2_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$$

- Use the statistics to greedily grow a tree $f_t(x)$

$$Obj = -\frac{1}{2} \sum_{j=1}^{T} \frac{G_j^2}{H_j + \lambda} + \gamma T$$

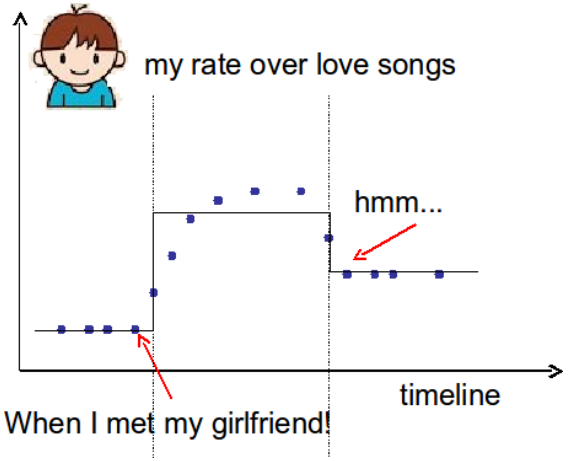
- Add $f_t(x)$ to the model $\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + f_t(x_i)$
  - Usually, instead we do $y^{(t)} = y^{(t-1)} + \epsilon f_t(x_i)$
  - ϵ is called step-size or shrinkage, usually set around 0.1
  - This means we do not do full optimization in each step and reserve chance for future rounds, it helps prevent overfitting

Outline

- Review of key concepts of supervised learning
- Regression Tree and Ensemble (What are we Learning)
- Gradient Boosting (How do we Learn)
- **Summary**

Questions to check if you really get it

- How can we build a boosted tree classifier to do weighted regression problem, such that each instance have a importance weight?
- Back to the time series problem, if I want to learn step functions over time. Is there other ways to learn the time splits, other than the top down split approach?



Questions to check if you really get it

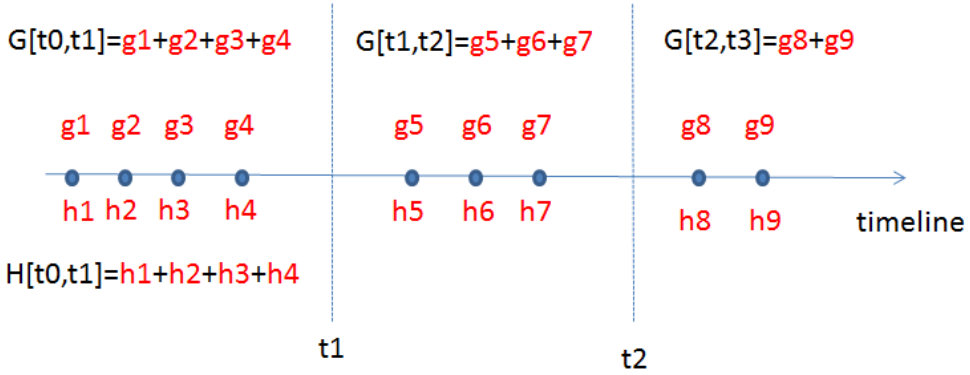
- How can we build a boosted tree classifier to do weighted regression problem, such that each instance have a importance weight?
  - Define objective, calculate g_i, h_i, feed it to the old tree learning algorithm we have for un-weighted version

$$l(y_i, \hat{y}_i) = \frac{1}{2} a_i (\hat{y}_i - y_i)^2 \qquad g_i = a_i(\hat{y}_i - y_i) \qquad h_i = a_i$$

  - Again think of separation of model and objective, how does the theory can help better organizing the machine learning toolkit

Questions to check if you really get it

- Time series problem



- All that is important is the structure score of the splits

$$Obj = -\frac{1}{2}\sum_{j=1}^{T}\frac{G_j^2}{H_j+\lambda} + \gamma T$$

  - Top-down greedy, same as trees
  - Bottom-up greedy, start from individual points as each group, greedily merge neighbors
  - Dynamic programming, can find optimal solution for this case

Summary

- The separation between model, objective, parameters can be helpful for us to understand and customize learning models
- The bias-variance trade-off applies everywhere, including learning in functional space

$$Obj(\Theta) = L(\Theta) + \Omega(\Theta)$$

- We can be formal about what we learn and how we learn. Clear understanding of theory can be used to guide cleaner implementation.

Reference

- Greedy function approximation a gradient boosting machine. *J.H. Friedman*
  - *First paper about gradient boosting*
- *Stochastic Gradient Boosting. J.H. Friedman*
  - *Introducing bagging trick to gradient boosting*
- *Elements of Statistical Learning. T. Hastie, R. Tibshirani and J.H. Friedman*
  - *Contains a chapter about gradient boosted boosting*
- Additive logistic regression a statistical view of boosting. *J.H. Friedman T. Hastie R. Tibshirani*
  - *Uses second-order statistics for tree splitting, which is closer to the view presented in this slide*
- Learning Nonlinear Functions Using Regularized Greedy Forest. *R. Johnson and T. Zhang*
  - *Proposes to do fully corrective step, as well as regularizing the tree complexity. The regularizing trick is closed related to the view present in this slide*
- Software implementing the model described in this slide: https://github.com/tqchen/xgboost